Electron Self-Energy and Generalized Drude Formula for Infrared Conductivity of Metals

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Götze and Wölfle (GW) wrote the conductivity in terms of a memory function $M(\omega)$ as $\sigma(\omega) = (ine^2/m)(\omega + M(\omega))^{-1}$, where $M(\omega) = i/\tau$ in the Drude limit. The analytic properties of $-M(\omega)$ are the same as those of the self-energy of a retarded Green's function. In the approximate treatment of GW, $-M$ closely resembles a self-energy, with differences, *e.g.*, the imaginary part is twice too large. The correct relation between $-M$ and Σ is known for the electron-phonon case and is conjectured to be similar for other perturbations. When vertex corrections are ignored there is a known relation. A derivation using Matsubara temperature Green's functions is given.

I. PRELIMINARIES

Holstein[1] used elementary arguments to show that in the infrared properties of metals there can be quantum effects (outside of the semiclassical Boltzmann approach) when the temperature is low enough and the probing frequency ω is degenerate with non-electronic excitations like phonons. Such effects have been seen experimentally[2,3]. Götze and Wölfle (GW)[4] gave a nice simplified way to compute such effects in the optical response of metals using truncated equations of motion to compute the "memory function" $M(\omega)$ defined as

$$\sigma(\omega) = \frac{ine^2/m}{\omega + M(\omega)} \tag{1}$$

In the dc limit, their formulas correctly reproduce lowest-order variational solutions of the corresponding Boltzmann transport theories. Unfortunately, a systematic perturbation theory for $M(\omega)$ is not known. The GW results are slightly less accurate than the corresponding lowest order results of Green's function theories.

The function $-M(\omega)$ has causal analytic properties and, not surprisingly, bears a close resemblance to an electron self-energy $\Sigma(\vec{k}, \omega)$ for $\vec{k}$-points averaged over the Fermi surface. However, the imaginary part of Σ is $-1/2\tau$ while the imaginary part of $-M$ must be $-1/\tau$. This is not the only difference between $-M$ and Σ. Since the analogy between $-M$ and Σ is sometimes used for analysis of infrared spectra[5], it is important to understand just how good it actually is. A full formula seems not to have been derived, and is beyond the ambition of this paper. A reasonable conjecture is that when anisotropy with k around the Fermi surface is not too important, then

$$\sigma(\omega) = \frac{ine^2}{m\omega} \int_{-\infty}^{\infty} d\omega' \frac{f(\omega') - f(\omega' + \omega)}{\omega - \Sigma_{\rm ir}(\omega' + \omega + i\eta) + \Sigma^*_{\rm ir}(\omega' + i\eta)}. \tag{2}$$

where $f(\omega') = (\exp(\beta\omega') + 1)^{-1}$ is the Fermi-Dirac function. Here $\Sigma_{\rm ir}$ is a modified version of Σ, averaged over the Fermi surface, with a complex weighting factor, similar to the familiar transport factor $1 - \cos(\theta)$. The actual weighting factor (in the solved electron-phonon case[6,7]) is found from a complex, frequency-dependent non-linear integral equation. Replacement of the weight factor by 1, turning $\Sigma_{\rm ir}$ into an ordinary, but $\vec{k}$-averaged, self-energy, should work fairly well in most cases. Sher[8] did a numerical study which tends to confirm that the difference between $\Sigma_{\rm ir}$ and Σ is small.

Eq. (2) implies a relation between $-M(\omega)$ and the self-energy which becomes more direct at low frequencies. Keeping the lowest order (in ω) terms, one gets a derivative of the Fermi-Dirac function $-\partial f(\omega')/\partial\omega'$ which can be approximated by the Dirac $\delta(\omega')$.

$$\begin{aligned} \sigma(\omega) &\approx \frac{ine^2}{m} \int_{-\infty}^{\infty} d\omega' \left(-\frac{\partial f(\omega')}{\partial \omega'} \right) \\ &\times \frac{1}{\omega(1 - d\Sigma_{\rm ir,1}(\omega')/d\omega') + 2i\Sigma_{\rm ir,2}(\omega')} \\ &\approx \frac{ine^2/m}{\omega - \omega d\Sigma_{\rm ir,1}(\omega)/d\omega + 2i\Sigma_{\rm ir,2}(\omega)} \end{aligned} \tag{3}$$

Therefore the real part of $-M$ at low frequencies is $\omega d{\rm Re}\Sigma_{\rm ir}(\omega)/d\omega$, and the imaginary part is $-2{\rm Im}\Sigma_{\rm ir}(\omega)$. If the interesting part of ${\rm Re}\Sigma$ is odd in ω, and approximately linear, then M at very low ω is a lot like Σ except for the factor of 2 in the imaginary part.

In the dc limit, the result $\sigma = ne^2\tau/m$ is retrieved, with $1/\tau = -2{\rm Im}\Sigma_{\rm ir}(\omega \to 0)$. There are minor differences between this and the more exact result found from a solution of the Boltzmann transport equation. These differences arise from $\vec{k}$-averaging and disappear for a spherical Fermi surface.

II. KUBO FORMULA

The starting point is the Kubo[9] formula for the conductivity. For external electric field $\vec{E}(t) = \vec{E}\cos(\omega t)$ the current operator $j = -e\sum_k v_{kx} c_k^\dagger c_k$ acquires a non-zero expectation value $j(t) = {\rm Re}[\sigma(\omega)\exp(-i\omega t)]E$, where the linear response coefficient $\sigma(\omega)$ is

$$\sigma(\omega) = \frac{i}{\omega}\left[r(\omega) + \frac{ne^2}{m} \right] \tag{4}$$

$$r(\omega) = i\int_0^\infty dt e^{i\omega t}\langle[j(t), j(0)]\rangle \quad (5)$$

The Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ has the non-interacting part $\mathcal{H}_0 = \sum_k \epsilon_k c_k^\dagger c_k$. The label k is short for the Bloch wavevector and other quantum numbers $(\vec{k}n\sigma)$. The state k has energy ϵ_k and group velocity $\vec{v}_k$.

To obtain a Wick-ordered perturbation theory we use an imaginary time $(0 \le \sigma \le \beta = 1/k_B T)$ version of $r(\omega)$,

$$r(i\omega_\mu) = -\int_0^\beta d\sigma e^{i\omega_\mu \sigma}\overline{\langle \hat{T} j(\sigma) j(0)\rangle} \quad (6)$$

where $j(\sigma) = \exp(\sigma\mathcal{H}) j \exp(-\sigma\mathcal{H})$. Angular brackets denote both a canonical ensemble temperature average and if necessary, an average over an ensemble of randomly distributed impurities. The Matsubara frequency ω_μ is $2\pi\mu/\beta$ and μ is an integer. When analytically continued from $i\omega_\mu$ to $\omega + i\eta$ just above the real ω axis (η is a positive infinitesimal) $r(i\omega_\mu)$ becomes $r(\omega)$, the retarded correlation function needed for the Kubo formula.

All Feynman graphs for $r(i\omega_\mu)$ are formally summed in terms of the exact electron Green's function

$$G(k, i\omega_\nu) = \frac{1}{i\omega_\nu - \epsilon_k - \Sigma(k, i\omega_\nu)}, \quad (7)$$

and the exact vertex function $\Gamma(k, k', i\omega_\mu, i\omega_\nu)$, where $\omega_\nu = 2\pi(\nu + 1/2)/\beta$. The exact answer is

$$\begin{aligned} r(i\omega_\mu) &= -\frac{e^2}{\beta}\sum_{kk'\nu} v_{k'x}\Gamma(kk', i\omega_\mu, i\omega_\nu) \\ &\times G(k, i\omega_\nu + i\omega_\mu) G(k, i\omega_\nu) \end{aligned} \quad (8)$$

Neither Σ nor Γ can be calculated exactly. A linearized Boltzmann equation is obtained when lowest order results for Σ and Γ are treated consistently.

An explicit formula relating σ to Σ occurs when Γ is replaced by its lowest order term,

$$\Gamma(kk', i\omega_\mu, i\omega_\nu) \rightarrow \Gamma_0 = v_{kx}\delta(k, k'). \quad (9)$$

The corresponding answer for $\sigma(\omega)$, denoted by $\sigma_0(\omega)$, after continuing to the real frequency axis, is

$$\sigma_0(\omega) = \frac{ine^2}{m\omega}\int_{-\infty}^\infty d\omega' \frac{f(\omega') - f(\omega' + \omega)}{\omega - \Sigma(\omega' + \omega + i\eta) + \Sigma^*(\omega' + i\eta)}. \quad (10)$$

This is not an original result, but since derivations are obscure, an elementary one is given in the next section.

Unlike the conjectured version Eq. (2), the approximation of Eq. (9) does not correctly reproduce the Boltzmann dc conductivity because of the omission of vertex corrections. The quasiparticle scattering rate $1/\tau = -2\mathrm{Im}\Sigma$ differs from the transport scattering rate $1/\tau_{\mathrm{tr}} = -2\mathrm{Im}\Sigma_{\mathrm{ir}}$ by the factor "$1 - \cos\theta$." This comes from scattering-in terms of the Boltzmann scattering operator, approximately the same as the contribution from the missing "rungs" of the vertex function omitted in Γ_0. The omitted correction takes into account that small angle θ scattering events do not degrade the current efficiently and make smaller contributions to $1/\tau_{\mathrm{tr}}$ than to $1/\tau$. The difference, except at low temperatures, is likely to be numerically small, since small angle scattering does not usually play a dominant role.

III. DERIVATION OF EQ. (10)

Starting by inserting Eq. (9) into Eq. (8),

$$r_0(i\omega_\mu) = -\frac{e^2}{\beta}\sum_k v_{kx}^2 G(k, i\omega_\nu + i\omega_\mu) G(k, i\omega_\nu) \quad (11)$$

This approximation, labeled r_0, keeps in principle arbitrarily complicated self-energy graphs in G.

The spectral function is defined as

$$G(k, i\omega_\nu) = \int_{-\infty}^\infty d\omega \frac{A(k, \omega)}{i\omega_\nu - \omega} \quad (12)$$

$$A(k, \omega) = -\frac{1}{\pi}\mathrm{Im}G(k, i\omega_\nu \rightarrow \omega + i\eta) \quad (13)$$

where $G(k, \omega + i\eta)$ is the "retarded" Green's function,

$$G(k, \omega + i\eta) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega)} \quad (14)$$

and $\Sigma(k, \omega) = \Delta(k, \omega) - i/2\tau(k, \omega)$ has imaginary part $1/2\tau$ non-negative. The approximate correlation function r_0 becomes

$$\begin{aligned} r_0(i\omega_\mu) &= -\frac{e^2}{\beta}\sum_k v_{kx}^2 \int_{-\infty}^\infty d\omega_1 \int_{-\infty}^\infty d\omega_2 A(k, \omega_1) A(k, \omega_2) \\ &\times \sum_\nu \left[\frac{1}{i\omega_\nu + i\omega_\mu - \omega_1}\ \frac{1}{i\omega_\nu - \omega_2}\right] \end{aligned} \quad (15)$$

The Matsubara sum can be performed exactly,

$$-\frac{1}{\beta}\sum_\nu \left[\frac{1}{i\omega_\nu + i\omega_\mu - \omega_1}\ \frac{1}{i\omega_\nu - \omega_2}\right] = \frac{f(\omega_2) - f(\omega_1)}{\omega_2 - \omega_1 + i\omega_\mu}. \quad (16)$$

The correlation function now is

$$\begin{aligned} r_0(i\omega_\mu) &= -e^2\int_{-\infty}^\infty d\epsilon \sum_k v_{kx}^2 \delta(\epsilon - \epsilon_k)\int_{-\infty}^\infty d\omega_1 \\ &\times \int_{-\infty}^\infty d\omega_2 A(k, \omega_1) A(k, \omega_2) \frac{f(\omega_2) - f(\omega_1)}{\omega_2 - \omega_1 + i\omega_\mu}, \end{aligned} \quad (17)$$

where a gratuitous factor $1 = \int d\epsilon\delta(\epsilon - \epsilon_k)$ was inserted. Because of the δ function in the k-sum

$$\sum_k v_{kx}^2 \delta(\epsilon - \epsilon_k) A(k, \omega_1) A(k, \omega_2) \quad (18)$$

it is allowed to replace ϵ_k in the denominators of the spectral functions by ϵ. There is a rapid dependence on

ϵ in $A(k,\omega)$ which must be treated carefully, and a remaining slow k dependence of $\Sigma(k,\omega)$ in the denominator of $A(k,\omega)$ which can be treated less carefully. The self-energies in the spectral functions $-(1/\pi)\mathrm{Im}(\omega-\epsilon_k-\Sigma)^{-1}$ are replaced by their k-average over the Fermi surface,

$$\Sigma(\omega) = \sum_k \Sigma(k,\omega)\delta(\epsilon_k)/\sum_k \delta(\epsilon_k). \tag{19}$$

This is usually not a bad approximation, because the anisotropy of $\Sigma(k,\omega)$, as $\vec{k}$ varies around the Fermi surface, is usually small. The errors introduced by doing this are of the same nature as the errors introduced by neglecting all vertex corrections. The k-sum is now

$$\begin{aligned}\sum_k v_{kx}^2\delta(\epsilon-\epsilon_k) &= \frac{1}{\hbar^2}\sum_k \frac{\partial\epsilon_k}{\partial k_x}\left(-\frac{\partial f}{\partial k_x}\right)\\ &= \frac{1}{\hbar^2}\sum_k \frac{\partial^2\epsilon_k}{\partial k_x^2} f = [n/m]_{\rm eff}(\epsilon).\end{aligned} \tag{20}$$

Here the δ function was replaced by $-\partial f/\partial\epsilon_k$. Integrating by parts gives the inverse effective mass $(\partial^2\epsilon_k/\partial k_x^2)/\hbar^2$ summed over all states lower in energy than ϵ.

The range of the remaining ϵ-integration is nominally $(-\infty,\infty)$. However, the factors $A(k,\omega)$ are peaked at $\epsilon=\omega_1$ and $\epsilon=\omega_2$; ω_1 and ω_2 thus have similar values. Because of the factor $(f(\omega_2)-f(\omega_1))$, they must both lie near the Fermi energy (one below and one above.) Therefore the ϵ integral is dominated by ϵ near the Fermi energy. The value of $[n/m]_{\rm eff}(\epsilon)$ at the Fermi energy is $[n/m]_{\rm eff}$, the number of electrons divided by the effective mass averaged over all states below the Fermi energy. An equivalent formula is

$$[n/m]_{\rm eff} = \sum_k v_{kx}^2\delta(\epsilon_k) = N(0) < v_x^2 > \tag{21}$$

The current correlation function now is

$$\begin{aligned}r_0(i\omega_\mu) &= \left[\frac{n}{m}\right]_{\rm eff} e^2\int_{-\infty}^{\infty}d\epsilon\int_{-\infty}^{\infty}d\omega_1\int_{-\infty}^{\infty}d\omega_2\\ &\times\ A(\epsilon,\omega_1)A(\epsilon,\omega_2)\frac{f(\omega_2)-f(\omega_1)}{\omega_2-\omega_1+i\omega_\mu}.\end{aligned} \tag{22}$$

It is necessary to integrate ϵ carefully over the Lorentzian peaks of $A(\epsilon,\omega_1)A(\epsilon,\omega_2)$. Cauchy's theorem can be used after closing the ϵ-contour by an arc going to infinity in either the upper or lower half-plane. The result is expressed by another identity,

$$\begin{aligned}&\int_{-\infty}^{\infty}d\epsilon\ \left(\tfrac{1}{\pi}\right)\ \mathrm{Im}\left(\frac{1}{\omega_1-\epsilon-\Sigma_1}\right)\left(\frac{1}{\pi}\right)\mathrm{Im}\left(\frac{1}{\omega_2-\epsilon-\Sigma_2}\right)\\ &\quad = -\left(\frac{1}{\pi}\right)\mathrm{Im}\left(\frac{1}{\omega_1-\omega_2-\Sigma_1+\Sigma_2^*}\right).\end{aligned} \tag{23}$$

The proof is elementary but tedious. The current correlation function is now

$$\begin{aligned}r_0(i\omega_\mu) &= \left[\frac{n}{m}\right]_{\rm eff}\frac{e^2}{\pi}\int_{-\infty}^{\infty}d\omega_1\int_{-\infty}^{\infty}d\omega_2\frac{f(\omega_2)-f(\omega_1)}{\omega_2-\omega_1+i\omega_\mu}\\ &\times\ \mathrm{Im}\left(\frac{1}{\omega_1-\omega_2-\Sigma_1+\Sigma_2^*}\right).\end{aligned} \tag{24}$$

The function $r_0(\omega)$ is now just $r_0(i\omega_\mu)$ with $i\omega_\mu$ replaced by $\omega+i\eta$. The only complex quantity in the formula for $r_0(\omega)$ is the factor $(\omega_2-\omega_1+\omega+i\eta)^{-1}$, so the real part $\mathrm{Re}\sigma_0(\omega)=\mathrm{Im}r_0(\omega)/\omega$ is

$$\begin{aligned}\mathrm{Re}\sigma_0(\omega) &= \left[\frac{n}{m}\right]_{\rm eff}\frac{e^2}{\omega}\int_{-\infty}^{\infty}d\omega_1\int_{-\infty}^{\infty}d\omega_2[f(\omega_2)-f(\omega_1)]\\ &\times\ \delta(\omega_2-\omega_1+\omega)\mathrm{Re}\left(\frac{i}{\omega_1-\omega_2-\Sigma_1+\Sigma_2^*}\right)\\ &= \left[\frac{n}{m}\right]_{\rm eff}e^2\int_{-\infty}^{\infty}d\omega'\left[\frac{f(\omega')-f(\omega'+\omega)}{\omega}\right]\\ &\times\ \mathrm{Re}\left(\frac{i}{\omega-\Sigma(\omega'+\omega)+\Sigma^*(\omega')}\right).\end{aligned} \tag{25}$$

The function $\sigma_0(\omega)$ is specified by the requirements of being analytic for $\mathrm{Im}\omega>0$, vanishing sufficiently rapidly as $\omega\to\infty$, and agreeing with Eq. (25). It is necessary and sufficient to remove the "real part" designator from both sides. This is the derivation of Eq. (10).

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